

Self-consistent initial conditions for primordial black hole formation

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Abstract

For an arbitrarily strong, spherically symmetric super-horizon curvature perturbation, we present analytic solutions of the Einstein equations in terms of the asymptotic expansion over the ratio of the Hubble radius to the length-scale of the curvature perturbation to set initial conditions for numerical computations of primordial black hole formation. To obtain this solution we develop a recursive method of quasi-linearization which reduces the problem to a system of coupled ordinary differential equations for the N th order terms in the asymptotic expansion with sources consisting of a non-linear combination of the lower order terms.

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I. INTRODUCTION

The idea that large-amplitude matter overdensities in the Universe could have collapsed through self-gravity to form primordial black holes (PBHs) was first put forward by Zel'dovich and Novikov [1], and then independently by Hawking [2], more than three decades ago. This theory suggests that large-amplitude inhomogeneities in the very early universe overcome internal pressure forces and collapse to form black holes. A lower threshold for the amplitude of such inhomogeneities was first provided by Carr [3, 4] for a radiation-dominated epoch. The PBH contribution to the energy density increases with time during this epoch. For this reason, the PBHs formed considerably before the end of radiation-domination, possibly even before radiation-domination [5], affect various cosmological and astrophysical processes even if their initial abundance is tiny. PBHs with mass smaller than $\sim 10^{15}\text{g}$ would have evaporated through Hawking radiation [6] and their abundances are constrained by big-bang nucleosynthesis [7–12] and the gamma-ray background [13–15], while holes with larger masses are constrained by dynamical and lensing effects [16] and by the stochastic gravitational wave background [17, 18]. All these constraints are updated and summarized in [19].

Since the probability of PBH formation depends crucially on the statistical characteristics of the random field of primordial perturbations, PBHs provide a useful and unique tool to obtain independent constraints on the primordial power spectrum of inhomogeneities on extremely small scales which cannot be probed by any other methods. To make this cosmological tool more reliable, we must improve the prescription of the initial conditions [20]. Self-consistent initial conditions are very important for calculations of the probability of PBH formation [21] and for relativistic hydrodynamical computations [22–25]. According to such computations the pressure gradients in the collapsing configuration play an extremely important role and are directly determined by the curvature profile in the initial configuration.

Since PBHs can form only from highly non-linear curvature perturbations, the initial conditions of their formation must be consistent with the underlying non-linear theory such as the general relativity. The main objective of the present paper is to exclude the possibility that even highly sophisticated computer simulations could produce irrelevant results due to inconsistency of the initial conditions. For example, if we assume that the Universe outside the configuration is spatially flat, the mass of a perturbed configuration of radius r should be equal to the mass of unperturbed sphere of the same radius. As a result, a self-consistent density profile should be non-monotonic, *i.e.* along with the region of density excess, it should contain a region of density deficit, which drastically changes the effect of pressure gradients [22].

For an arbitrarily strong spherically symmetric super-horizon curvature perturbation, we present an analytic solution of the Einstein equations in terms of an asymptotic expansion over the ratio of the Hubble radius to the length-scale of the curvature perturbation under consideration. This method is similar to the gradient expansion [26–31] (previously known as the anti-Newtonian expansion [32]) in spirit, but thanks to the spherical symmetry we can construct a solution to arbitrary higher order in this ratio from a single function characterising the curvature profile. Note that the lowest-order solution in this program has been obtained in [20, 22, 33]. Here we develop the recursive method of quasi-linearization which reduces the problem to a system of coupled ordinary differential equations for terms of n th order in the asymptotic expansion of the density, pressure, velocity and metric, with sources which contain a non-linear combination of the lower order terms. Using this method, we obtain analytic expressions for all terms.

The curvature profile, $K_1(r)$, to be defined below, appears in the source terms on the right-hand side of the relevant equations and deviations from homogeneity in density and velocity are

generated by the inhomogeneity of the curvature. To avoid confusion, we should say that these deviations do not involve small cosmological perturbations at all. Statistical characteristics of small perturbations are only relevant in this context when one calculates the probability of finding a configuration with a high amplitude perturbation of the metric.

Dropping all terms of order greater than N , we obtain truncated asymptotic solutions of N th order. Then for the arbitrary precision required by the intended accuracy and stability of the computer code, we obtain an upper limit on the time when such an N th order truncated expansion can be used to set the initial conditions of fully non-linear numerical simulations of PBH formation. Later initial times obviously correspond to shorter computer runs. Thus our analytic solution helps to optimize numerical computations.

The rest of the paper is organized as follows. In §II basic equations are derived and in §III expansion coefficients are defined and their properties are described. Then in §IV we derive the recursive formulae for the coefficients in our problem and they are solved in §V for several specific initial curvature profiles. §VI is devoted to discussion and drawing conclusions.

II. MATHEMATICAL FORMULATION OF THE PROBLEM

A. The Misner-Sharp equations

Assuming spherical symmetry, it is convenient to divide the collapsing matter into a system of concentric spherical shells and to label each shell with a Lagrangian comoving radial coordinate r . Then the metric can be written in the form used by Misner and Sharp [34]:

$$ds^2 = -a^2 dt^2 + b^2 dr^2 + R^2(d\theta^2 + \sin^2\theta d\phi^2), \quad (1)$$

where R , a and b are functions of r and the time coordinate t . We consider a perfect fluid with energy density $\rho(r, t)$ and pressure $p(r, t)$ and constant equation-of-state parameter γ , $p(r, t) = \gamma\rho(r, t)$. Expressing the proper time derivative of R as

$$u \equiv \frac{\dot{R}}{a}, \quad (2)$$

with a dot denoting a derivative with respect to t , we derive equations of motion for these variables as follows.

First, from the $(\frac{0}{r})$ component of the Einstein equations, we find

$$\frac{\dot{b}}{b} = \frac{au'}{R'}, \quad (3)$$

while the Euler equation yields

$$\frac{a'}{a} = -\frac{\gamma}{1+\gamma} \frac{\rho'}{\rho}, \quad (4)$$

where a prime denotes differentiation with respect to r . We define the mass within the shell of proper radius R by

$$M(r, t) = 4\pi \int_0^{R(r, t)} \rho(r, t) R^2 dR, \quad (5)$$

which gives

$$M' = 4\pi\rho R^2 R'. \quad (6)$$

Using (3), the (0) component of the Einstein equations becomes

$$\frac{R'^2}{b^2} = 1 + u^2 - \frac{2GM}{R}, \quad (7)$$

and (5) can then be expressed as

$$M(r, t) = \int_0^r \rho \left(1 + u^2 - \frac{2GM}{R} \right)^{\frac{1}{2}} dV, \quad (8)$$

where $dV \equiv 4\pi R^2 b dr$ is the proper volume element. Equation (8) shows that M includes contributions from both the kinetic energy and the gravitational potential energy. Finally, combining (3)~(7), the evolution equation of M becomes

$$\dot{M} = -4\pi p R^2 \dot{R}. \quad (9)$$

B. Quasi-homogenous asymptotic equations in new variables

We consider the evolution of a perturbed region described by the above equations embedded in a flat Friedmann-Lemaitre-Robertson-Walker (FLRW) Universe with metric

$$ds^2 = -dt^2 + S^2(t)(dr^2 + r^2 d\theta^2 + r^2 \sin^2 \theta d\phi), \quad (10)$$

which is a particular case of (1). The scale factor in this background evolves as

$$S(t) = \left(\frac{t}{t_i} \right)^\alpha, \quad \alpha \equiv \frac{2}{3(1+\gamma)}, \quad (11)$$

where t_i is some reference time.

We denote the background solution with a suffix 0. In terms of the metric variables defined in (1), we find

$$a_0 = 1, \quad b_0 = S(t), \quad R_0 = rS(t). \quad (12)$$

The background Hubble parameter is

$$H_0(t) = \frac{\dot{R}_0}{a_0 R_0} = \frac{\dot{S}}{S} = \frac{\alpha}{t}, \quad (13)$$

and the energy density is calculated from the Friedmann equation,

$$\rho_0(t) = \frac{3\alpha^2}{8\pi G t^2}. \quad (14)$$

We introduce a variable H defined by

$$H(t, r) \equiv \frac{\dot{R}}{aR} = \frac{u}{R} \quad (15)$$

and another new variable \tilde{H} by rewriting H as

$$H(t, r) = H_0(t) \tilde{H}(t, r). \quad (16)$$

The tilde-variable \tilde{H} , as well as most of the other tilde-variables introduced below, represent deviations of the solutions from the corresponding ones in the flat FLRW universe. Specifically we find

$$a(t, r) = a_0(t) \tilde{a}(t, r) = \tilde{a}(t, r), \quad (17)$$

$$b(t, r) = b_0(t)\tilde{b}(t, r) = S(t)\tilde{b}(t, r), \quad (18)$$

$$R(t, r) = R_0(t)\tilde{R}(t, r) = rS(t)\tilde{R}(t, r), \quad (19)$$

$$\rho(t, r) = \rho_0(t)\tilde{\rho}(t, r) \propto t^{-4\alpha}\tilde{\rho}. \quad (20)$$

We define another variable $\tilde{\mu}$ by

$$M = \frac{4\pi}{3}\rho_0 R^3 \tilde{\mu}, \quad (21)$$

and the curvature profile $K(t, r)$ is defined by rewriting b as

$$b(t, r) = \frac{R'(t, r)}{\sqrt{1 - K(t, r)r^2}}. \quad (22)$$

$K(t, r)$ vanishes outside the perturbed region so that the solution asymptotically approaches the background FLRW solution at spatial infinity.

We denote the comoving radius of a perturbed region by r_i , whose precise definition will be given later, and define a dimensionless parameter ϵ in terms of the square ratio of the Hubble radius H_0^{-1} to the physical length scale of the configuration,

$$\epsilon \equiv \left(\frac{H_0^{-1}}{S(t)r_i} \right)^2 = (\dot{S}r_i)^{-2} = \frac{t_i^{2\alpha}t^\beta}{\alpha^2 r_i^2}, \quad \beta \equiv 2(1 - \alpha). \quad (23)$$

When we set the initial conditions for PBH formation, the size of the perturbed region is much larger than the Hubble horizon. This remains the case until the horizon mass becomes larger than the PBH mass. The horizon mass grows with cosmic time (for the radiation-dominated regime, the growth is directly proportional to time). This means $\epsilon \ll 1$ at the beginning, so it can serve as an expansion parameter to construct an analytic solution of the system (2)-(7) to describe the dependence of all the above variables on the initial moment at which we set initial conditions. For the sake of brevity, below we will call this dependence “time evolution”.

For our analytic expansion, it is convenient to rewrite the system of equations (2)-(7) in terms of the tilde-variables, all of which tend to 1 at spatial infinity. From (4), we find

$$\frac{\tilde{a}'}{\tilde{a}} + \frac{\gamma}{1 + \gamma} \frac{\tilde{\rho}'}{\tilde{\rho}} = [\ln(\tilde{a}\tilde{\rho}^{\frac{\gamma}{1+\gamma}})]' = 0, \quad (24)$$

so

$$\tilde{a} = F(t)\tilde{\rho}^{-\frac{\gamma}{1+\gamma}}, \quad (25)$$

where $F(t)$ is an arbitrary function of time. For convenience we choose $F(t) = 1$, then

$$\tilde{a} = \tilde{\rho}^{-\frac{\gamma}{1+\gamma}}. \quad (26)$$

Such a choice of $F(t)$ corresponds to a frame of reference which is synchronous at spatial infinity.

Since both $\tilde{\rho}$ and \tilde{a} are positive definite, we may define $\hat{\rho} \equiv \ln \tilde{\rho}$ and $\hat{a} \equiv \ln \tilde{a}$ and then rewrite (26) as

$$\hat{a} = -\frac{\gamma}{1 + \gamma} \hat{\rho}. \quad (27)$$

Using the tilde-variables, we can rewrite (2) as

$$\alpha\tilde{R} + t\dot{\tilde{R}} = \alpha\tilde{a}\tilde{H}\tilde{R}, \quad (28)$$

so

$$t\dot{\tilde{R}} = \alpha\tilde{R}(\tilde{\Phi} - 1), \quad (29)$$

where

$$\tilde{\Phi} \equiv \tilde{a}\tilde{H}. \quad (30)$$

Since \tilde{R} is positive, we can also define \hat{R} by $\hat{R} \equiv \ln \tilde{R}$. Introducing a new time variable

$$\xi \equiv \ln \left(\frac{t}{t_i} \right), \quad (31)$$

(29) is expressed as

$$\frac{\partial \hat{R}}{\partial \xi} = \alpha(\tilde{\Phi} - 1). \quad (32)$$

From the definition of the curvature profile function $K(r, t)$, (22), we find

$$-r^2 \dot{K} = \left(\frac{R'^2}{b^2} \right)' = \frac{2R'^2}{b^2} \left(\frac{\dot{R}'}{R'} - \frac{\dot{b}}{b} \right) = 2(1 - Kr^2) \left(\frac{\dot{R}'}{R'} - \frac{\dot{b}}{b} \right). \quad (33)$$

Using (2) and (3), this can be rewritten as

$$-r^2 \dot{K} = 2H(1 - Kr^2) \frac{a'r\tilde{R}}{(r\tilde{R})'} \equiv 2H(1 - Kr^2) D_r \tilde{a}, \quad (34)$$

where we have introduced the operator

$$D_r \equiv \frac{r\tilde{R}\partial}{(r\tilde{R})'\partial r}. \quad (35)$$

We write the initial condition for (34) as

$$K(0, r) \equiv K_i(r), \quad (36)$$

where $K_i(r)$ is an arbitrary function of r which vanishes outside the perturbed region, and define a new variable \tilde{K} by

$$1 - K(t, r)r^2 = (1 - K_i(r)r^2)\tilde{K}(t, r). \quad (37)$$

\tilde{K} is unity at spatial infinity like the other tilde-variables, but in contrast to the other tilde-variables, it describes the evolution of curvature deviation from the initial curvature profile rather than the deviation from the spatially flat Friedmann universe. Note that, from the definition (22) of $b(t, r)$, $K_i(r)$ has to satisfy the condition

$$K_i(r) < \frac{1}{r^2}. \quad (38)$$

Physically, this condition ensures that the perturbed region does not form a closed universe which is causally disconnected from our universe [35, 36].

Differentiating (37) with respect to t and using (34), we find

$$(1 - K_i r^2) \dot{\tilde{K}} = -r^2 \dot{K} = 2H(1 - Kr^2) D_r \tilde{a} = 2H(1 - K_i r^2) \tilde{K} D_r \tilde{a}, \quad (39)$$

which yields

$$t \dot{\tilde{K}} = 2\alpha \tilde{H} \tilde{K} D_r \tilde{a}. \quad (40)$$

Since \tilde{K} is always positive, we can define another hat variable, $\hat{K} \equiv \ln \tilde{K}$, and rewrite (40) using (26) as

$$\frac{\partial \hat{K}}{\partial \xi} = 2\alpha \tilde{H} D_r \tilde{a} = -\frac{2\alpha\gamma\tilde{\Phi}}{1+\gamma} \frac{D_r \tilde{\rho}}{\tilde{\rho}} = -\frac{4\gamma}{3(1+\gamma)^2} \tilde{\Phi} D_r \hat{\rho}. \quad (41)$$

Using (21), we can write (6) in terms of the tilde-variables as

$$\frac{4\pi}{3}\rho_0 R^3 \tilde{\mu} \left(\frac{\tilde{\mu}'}{\tilde{\mu}} + 3 \frac{(r\tilde{R})'}{r\tilde{R}} \right) = 4\pi\rho R^3 \frac{(r\tilde{R})'}{r\tilde{R}}, \quad (42)$$

which leads to

$$\tilde{\mu}' + 3\tilde{\mu} \frac{(r\tilde{R})'}{r\tilde{R}} = 3\tilde{\rho} \frac{(r\tilde{R})'}{r\tilde{R}} \quad (43)$$

and hence

$$\tilde{\rho} = \tilde{\mu} + \frac{1}{3}D_r\tilde{\mu}. \quad (44)$$

In terms of the tilde-variables, (9) can be written as

$$\dot{\tilde{\mu}} + \tilde{\mu} \left(-\frac{2}{t} + 3\frac{\dot{R}}{R} \right) + 3\gamma \frac{\rho}{\rho_0} \frac{\dot{R}}{R} = 0, \quad (45)$$

so

$$t\dot{\tilde{\mu}} = 2\tilde{\mu} - 3\alpha\tilde{a}\tilde{H}(\tilde{\mu} + \gamma\tilde{\rho}). \quad (46)$$

Defining

$$\tilde{f} \equiv \frac{\tilde{\mu} + \gamma\tilde{\rho}}{1 + \gamma}, \quad (47)$$

(46) can be rewritten as

$$\frac{\partial \tilde{\mu}}{\partial \xi} = 2(\tilde{\mu} - \tilde{\Phi}\tilde{f}). \quad (48)$$

In terms of H , the constraint equation (7) is expressed as

$$H^2 = \frac{8\pi G}{3}\rho_0\tilde{\mu} - \frac{Kr^2}{R^2} \quad (49)$$

and this gives

$$\tilde{\mu} = \tilde{H}^2 + \frac{\epsilon Kr_i^2}{\tilde{R}^2}. \quad (50)$$

One important property of the perturbation follows from (49) and the boundary conditions. The equation (49) corresponds to the Friedmann equation of the flat FLRW universe

$$H_0^2 = \frac{8\pi G}{3}\rho_0. \quad (51)$$

Using (5) and (21), (49) and (51) are combined to give

$$\frac{H^2 - H_0^2}{H_0^2} = 4\pi \int_0^R \left(\frac{\rho - \rho_0}{\rho_0} \right) R^2 dR - \frac{Kr^2}{R^2 H_0^2}. \quad (52)$$

Noting the left-hand side and the second term of the right-hand side vanish at spatial infinity as a result of the boundary conditions and defining the energy density perturbation

$$\delta(t, r) \equiv \frac{\rho(t, r) - \rho_0(t)}{\rho_0(t)} = \tilde{\rho}(t, r) - 1, \quad (53)$$

(52) leads to the following condition for δ :

$$4\pi \int_0^\infty \delta R^2 dR = 0. \quad (54)$$

Namely, the mass excess in the center has to be compensated by the surrounding mass deficit in order for the solution to coincide with the flat FLRW solution at spatial infinity.

Equations (26), (32), (41), (44), (48) and (50) are the fundamental equations to solve.

III. EXPANSION OVER ϵ AND QUASI-LINEARIZATION

We now expand the tilde-variables over the parameter ϵ as a first step to solving these fundamental equations:

$$\tilde{X}(t, r) = \sum_{n=0}^{\infty} \epsilon^n(t) \tilde{X}_{(n)}(r). \quad (55)$$

Note that by definition $\tilde{X}_{(0)} = 1$ and $\tilde{X}'_{(0)} = 0$. The hat-variables are expanded similarly. Differentiating this expansion with respect to t , one obtains

$$\dot{\tilde{X}}(t, r) = \dot{\epsilon} \sum_{n=0}^{\infty} n \epsilon^{n-1}(t) \tilde{X}_{(n)}(r) = \frac{\beta}{t} \sum_{n=1}^{\infty} n \epsilon^n(t) \tilde{X}_{(n)}(r), \quad (56)$$

hence

$$\left(\dot{\tilde{X}} \right)_{(n)} = \frac{n\beta}{t} \tilde{X}_{(n)}. \quad (57)$$

Differentiating the expansion with respect to r , one finds

$$\tilde{X}'(t, r) = \sum_{n=1}^{\infty} \epsilon^n(t) \tilde{X}'_{(n)}(r), \quad (58)$$

hence

$$(\tilde{X}')_{(n)} = \tilde{X}'_{(n)}. \quad (59)$$

Let us consider the product of two tilde-variables \tilde{X}_1 and \tilde{X}_2 :

$$\tilde{X}_1 \tilde{X}_2 = \left(\sum_{i=0}^{\infty} \epsilon^i \tilde{X}_{1(i)} \right) \left(\sum_{j=0}^{\infty} \epsilon^j \tilde{X}_{2(j)} \right) = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \epsilon^{i+j} \tilde{X}_{1(i)} \tilde{X}_{2(j)}, \quad (60)$$

from which one finds

$$(\tilde{X}_1 \tilde{X}_2)_{(n)} = \sum_{i=0}^n \tilde{X}_{1(i)} \tilde{X}_{2(n-i)}. \quad (61)$$

Since $\tilde{X}_{1(0)} = \tilde{X}_{2(0)} = 1$, one obtains

$$(\tilde{X}_1 \tilde{X}_2)_{(n)} = \tilde{X}_{1(n)} + \tilde{X}_{2(n)} + S_{(n)}[\tilde{X}_1 \tilde{X}_2], \quad (62)$$

where

$$S_{(n)}[\tilde{X}_1 \tilde{X}_2] \equiv \sum_{i=1}^{n-1} \tilde{X}_{1(i)} \tilde{X}_{2(n-i)}. \quad (63)$$

Note that $S_{(0)}[\tilde{X}_1 \tilde{X}_2] = S_{(1)}[\tilde{X}_1 \tilde{X}_2] = 0$. The most important feature of $S_{(n)}[\tilde{X}_1 \tilde{X}_2]$ is that it depends only on coefficients up to $(n-1)$ th order.

The relationship (62) can be generalized to arbitrary functions of the tilde-variables. Let F_1 and F_2 be arbitrary functions of tilde-variables and their time and space derivatives. Then

$$(F_1 F_2)_{(n)} = \sum_{i=0}^n F_{1(i)} F_{2(n-i)} = F_{1(n)} F_{2(0)} + F_{1(0)} F_{2(n)} + S_{(n)}[F_1 F_2]. \quad (64)$$

As a consequence of (59) and (64), since $\tilde{X}'_{i(0)} = 0$, one finds

$$(\tilde{X}' F)_{(n)} = \tilde{X}'_{(n)} F_{(0)} + S_{(n)}[(\tilde{X}')' F], \quad (65)$$

and

$$(\tilde{X}_1' \tilde{X}_2')_{(n)} = S_{(n)}[(\tilde{X}_1')(\tilde{X}_2')]. \quad (66)$$

Similarly, using (57) and (64) and noting $\dot{\tilde{X}}_{(0)} = 0$, one obtains

$$(\dot{\tilde{X}}F)_{(n)} = \frac{n\beta}{t} \tilde{X}_{(n)} F_{(0)} + S_{(n)}[(\dot{\tilde{X}})F] = \frac{n\beta}{t} \left(\tilde{X}_{(n)} F_{(0)} + \frac{1}{n} S_{(n)}^*[\tilde{X}F] \right), \quad (67)$$

where we have defined

$$S_{(n)}^*[\tilde{X}F] = \sum_{m=1}^{n-1} m \tilde{X}_m F_{(n-m)}. \quad (68)$$

We also find

$$(\dot{\tilde{X}}_1 \tilde{X}_2')_{(n)} = \frac{\beta}{t} S_{(n)}^*[\tilde{X}_1 \tilde{X}_2']. \quad (69)$$

It is useful to obtain relationships between the expansion coefficients of the tilde-variables and those of the hat-variables. Suppose \tilde{Y} is some product of the positive-definite quantities $\tilde{a}, \tilde{R}, \tilde{\rho}$ and \tilde{K} , such as

$$\tilde{Y} \equiv \tilde{a}^{p_1} \tilde{R}^{p_2} \tilde{\rho}^{p_3} \tilde{K}^{p_4}, \quad (70)$$

where p_1, \dots, p_2 are integers. Then defining

$$\hat{Y} \equiv \ln \tilde{Y} = p_1 \hat{a} + p_2 \hat{R} + p_3 \hat{\rho} + p_4 \hat{K}, \quad (71)$$

we can relate the expansion coefficients of

$$\tilde{Y}_{(n)} = \frac{1}{n!} \lim_{\epsilon \rightarrow 0} \frac{\partial^n \tilde{Y}}{\partial \epsilon^n} \quad (72)$$

and

$$\hat{Y}_{(n)} = \frac{1}{n!} \lim_{\epsilon \rightarrow 0} \frac{\partial^n \hat{Y}}{\partial \epsilon^n}, \quad (73)$$

by

$$\begin{aligned} \tilde{Y}_{(n)} &= \frac{1}{n} \sum_{m=1}^n \frac{m!}{(m-1)!} \lim_{\epsilon \rightarrow 0} \left(\frac{\partial^m \hat{Y}}{m! \partial \epsilon^m} \right) \lim_{\epsilon \rightarrow 0} \left(\frac{\partial^{n-m}}{(n-m)! \partial \epsilon^{n-m}} e^{\hat{Y}} \right) \\ &= \frac{1}{n} \sum_{m=1}^n m \hat{Y}_{(m)} \tilde{Y}_{(n-m)}. \end{aligned} \quad (74)$$

Using $\tilde{Y}_{(0)} = 1$, we obtain

$$\tilde{Y}_{(n)} = \hat{Y}_{(n)} + \frac{1}{n} S_{(n)}^*[\hat{Y} \tilde{Y}]. \quad (75)$$

IV. EQUATIONS FOR ANALYTIC CALCULATIONS

The fundamental equations to be solved in the following are (27), (32), (41), (44), (48) and (50). We solve for the expansion coefficients $X_{i(n)}$ of each tilde or hat variable in the power series expansion with respect to ϵ using these equations. To do this, we derive a set of recursive formulae to express $X_{i(n)}$ in terms of $X_{j(m)}$ with $m < n$.

First from (27) we find

$$\hat{a}_{(n)} = -\frac{\gamma}{1+\gamma} \hat{\rho}_{(n)}, \quad (76)$$

which yields

$$(1 + \gamma)\tilde{a}_{(n)} + \gamma\tilde{\rho}_{(n)} = \frac{\gamma}{n}S_{(n)}^*[\hat{\rho}(\tilde{\rho} - \tilde{a})]. \quad (77)$$

From (48) and (50) with (77), we can express $\tilde{H}_{(n)}$ and $\tilde{\mu}_{(n)}$ in terms of the lower-order coefficients as follows. Using (62), (64) and (75), (50) leads to

$$\begin{aligned} \tilde{\mu}_{(n)} - 2\tilde{H}_{(n)} &= S_{(n)}[\tilde{H}\tilde{H}] + \frac{r_i^2}{r^2}(e^{-2\hat{R}})_{(n-1)} \\ &+ r_i^2 \left(K_i - \frac{1}{r^2} \right) \left\{ (e^{\hat{K}})_{(n-1)} + (e^{-2\hat{R}})_{(n-1)} + S_{(n-1)}[e^{\hat{K}}e^{-2\hat{R}}] \right\} \\ &\equiv F_{(n)} + W_{1(n)} \end{aligned} \quad (78)$$

where

$$F_{(n)} \equiv \delta_n^1 r_i^2 K_i - 2r_i^2 K_i \hat{R}_{(n-1)} + r_i^2 \left(K_i - \frac{1}{r^2} \right) \hat{K}_{(n-1)}, \quad (79)$$

and

$$\begin{aligned} W_{1(n)} &\equiv S_{(n)}[\tilde{H}\tilde{H}] + r_i^2 \left(K_i - \frac{1}{r^2} \right) S_{(n-1)}[e^{\hat{K}}e^{-2\hat{R}}] \\ &+ \frac{1}{n-1} \left\{ r_i^2 \left(K_i - \frac{1}{r^2} \right) S_{(n-1)}^*[\hat{K}e^{\hat{K}}] - 2r_i^2 K_i S_{(n-1)}^*[\hat{R}e^{-2\hat{R}}] \right\}. \end{aligned} \quad (80)$$

On the other hand, (48) yields

$$n\beta\tilde{\mu}_{(n)} = 2\tilde{\mu}_{(n)} - 2(\tilde{\Phi}\tilde{f})_{(n)}. \quad (81)$$

Using the equalities

$$\tilde{\Phi}_{(n)} = \tilde{a}_{(n)} + \tilde{H}_{(n)} + S_{(n)}[\tilde{a}\tilde{H}], \quad (82)$$

$$\tilde{f}_{(n)} = \frac{1}{1+\gamma}(\gamma\tilde{\rho}_{(n)} + \tilde{\mu}_{(n)}), \quad (83)$$

we find

$$\begin{aligned} (\tilde{\Phi}\tilde{f})_{(n)} &= \tilde{a}_{(n)} + \tilde{H}_{(n)} + S_{(n)}[\tilde{a}\tilde{H}] + \frac{1}{1+\gamma}(\tilde{\mu}_{(n)} + \gamma\tilde{\rho}_{(n)}) + S_{(n)}[\tilde{\Phi}\tilde{f}] \\ &= \tilde{H}_{(n)} + \frac{1}{1+\gamma}\tilde{\mu}_{(n)} + \frac{\gamma}{(1+\gamma)n}S_{(n)}^*[\hat{\rho}(\tilde{\rho} - \tilde{a})] \\ &+ S_{(n)}[\tilde{a}\tilde{H}] + S_{(n)}[\tilde{\Phi}\tilde{f}], \end{aligned} \quad (84)$$

where we have used (77) in the last equality. From (78) and (84) we have

$$\tilde{\mu}_{(n)} = \frac{1}{1+A_n}(F_{(n)} + W_{1(n)} - W_{2(n)}), \quad (85)$$

$$\tilde{H}_{(n)} = -\frac{1}{2(1+A_n)}[A_n(F_{(n)} + W_{1(n)}) + W_{2(n)}], \quad (86)$$

where

$$A_n \equiv \frac{2}{1+\gamma} \left[\left(\gamma + \frac{1}{3} \right) n - \gamma \right], \quad (87)$$

$$W_{2(n)} \equiv 2 \left(S_{(n)}[\tilde{a}\tilde{H}] + S_{(n)}[\tilde{\Phi}\tilde{f}] + \frac{\gamma}{n(1+\gamma)}S_{(n)}^*[\hat{\rho}(\tilde{\rho} - \tilde{a})] \right). \quad (88)$$

Now that we have expressed $\tilde{\mu}_{(n)}$ and $\tilde{H}_{(n)}$ in terms of lower-order coefficients, we may use these coefficients to obtain recursive formulae for the other variables. For example, from (44) we find

$$\tilde{\rho}_{(n)} = \tilde{\mu}_{(n)} + \frac{r}{3}\tilde{\mu}'_{(n)} + W_{3(n)}, \quad (89)$$

with

$$W_{3(n)} \equiv S_{(n)}[(\tilde{\mu} - \tilde{\rho})(r\tilde{R})'] + \frac{r}{3}S_{(n)}[\tilde{\mu}'\tilde{R}], \quad (90)$$

where we have used (65). Then from (77) we find

$$\tilde{a}_{(n)} = -\frac{\gamma}{1+\gamma} \left(\tilde{\mu}_{(n)} + \frac{r}{3}\tilde{\mu}'_{(n)} \right) + W_{4(n)}, \quad (91)$$

with

$$W_{4(n)} \equiv -\frac{\gamma}{1+\gamma}W_{3(n)} + \frac{\gamma}{(1+\gamma)n}S_{(n)}^*[\hat{\rho}(\tilde{\rho} - \hat{a})]. \quad (92)$$

Similarly (32) yields

$$\hat{R}_{(n)} = \frac{1}{(1+3\gamma)n}(\tilde{a}_{(n)} + \tilde{H}_{(n)} + W_{5(n)}), \quad (93)$$

with

$$W_{5(n)} \equiv S_{(n)}[\tilde{a}\tilde{H}]. \quad (94)$$

From (41)

$$\hat{K}_{(n)} = -\frac{2\gamma}{(1+\gamma)(1+3\gamma)n}(r\hat{\rho}'_{(n)} + W_{6(n)}), \quad (95)$$

with

$$W_{6(n)} \equiv rS_{(n)}[\hat{\rho}'(\tilde{\Phi}\tilde{R})] + \left(2 + \frac{1}{2\gamma} + \frac{3\gamma}{2}\right) S_{(n)}^*[\hat{K}(r\tilde{R})']. \quad (96)$$

The corresponding tilde-variables are obtained from

$$\tilde{R}_{(n)} = \hat{R}_{(n)} + \frac{1}{n}S_{(n)}^*[\hat{R}\tilde{R}], \quad (97)$$

$$\tilde{K}_{(n)} = \hat{K}_{(n)} + \frac{1}{n}S_{(n)}^*[\hat{K}\tilde{K}]. \quad (98)$$

This completes our derivation of the recursive formulae. The first-order coefficients are determined by the initial profile of the curvature inhomogeneity $K_i(r)$ as

$$\tilde{\mu}_{(1)}(r) = \frac{3(1+\gamma)r_i^2K_i(r)}{5+3\gamma}, \quad (99)$$

$$\tilde{H}_{(1)}(r) = -\frac{r_i^2K_i(r)}{5+3\gamma}, \quad (100)$$

$$\tilde{\rho}_{(1)}(r) = \frac{(1+\gamma)r_i^2(3K_i(r) + rK_i'(r))}{5+3\gamma}, \quad (101)$$

$$\tilde{a}_{(1)}(r) = -\frac{\gamma r_i^2(3K_i(r) + rK_i'(r))}{5+3\gamma}, \quad (102)$$

$$\tilde{R}_{(1)}(r) = -\frac{(1+3\gamma)r_i^2K_i(r) + \gamma r_i^2rK_i'(r)}{5+18\gamma+9\gamma^2}, \quad (103)$$

$$\tilde{K}_{(1)}(r) = -\frac{2\gamma r_i^2r(4K_i'(r) + rK_i''(r))}{(1+3\gamma)(5+3\gamma)}. \quad (104)$$

V. ANALYTIC SOLUTION

Dropping all terms of order greater than N , we obtain truncated asymptotic solutions of N th order. In order to use these solutions to set the initial conditions of numerical simulation of PBH formation, it is necessary to estimate an upper limit on time when such solutions are accurate enough to be used. Let the maximum acceptable error of the analytic solution be Δ . Then the latest epoch for which the analytic solution is accurate enough is determined by the first dropped terms of the truncated asymptotic expansions. If we use the asymptotic expansion of N th order, the error of the asymptotic expansion for \tilde{X} is

$$\text{ERR} \left(\sum_{n=0}^N \epsilon^n \tilde{X}_{(n)} \right) \equiv \tilde{X} - \sum_{n=0}^N \epsilon^n \tilde{X}_{(n)} = O(\epsilon^{N+1} \tilde{X}_{(N+1)}). \quad (105)$$

Then we require

$$\epsilon^{N+1} M_{(N+1)} < \Delta, \quad (106)$$

where $M_{(n)}$ and $M_{\tilde{X}_{(n)}}$ are defined by

$$M_{(n)} \equiv \max \left\{ M_{\tilde{a}_{(n)}}, M_{\tilde{R}_{(n)}}, M_{\tilde{K}_{(n)}}, M_{\tilde{\rho}_{(n)}}, M_{\tilde{\mu}_{(n)}}, M_{\tilde{H}_{(n)}} \right\} \quad (107)$$

and

$$M_{\tilde{X}_{(n)}} \equiv \max_r |\tilde{X}_{(n)}(r)|, \quad (108)$$

respectively. The error associated with the analytic calculation is less than Δ if it is calculated when

$$\epsilon < \epsilon_{\text{max}} \equiv \sqrt[N+1]{\frac{\Delta}{M_{(N+1)}}}. \quad (109)$$

We solve the recursive relations obtained in §IV for four specific curvature profiles of the form

$$K_i(r) = \left[1 + \frac{B}{2} \left(\frac{r}{\sigma} \right)^2 \right] \exp \left[-\frac{1}{2} \left(\frac{r}{\sigma} \right)^2 \right], \quad (110)$$

where B describes slope of curvature profiles and σ specifies the comoving length scale of curvature profile. Smaller values of B correspond to shallower profiles, and when $B = 0$ the profile is simply Gaussian. The amplitude of the profile is set to unity at the origin where the same normalization is used as a spatially closed Friedmann universe in accordance with [20].

In order to represent the comoving length scale of the perturbed region, we use the comoving radius, r_i , of the overdense region. We can calculate r_i by solving the following equation for the energy density perturbation defined by (53):

$$\delta(t, r_i) = 0. \quad (111)$$

Since the initial condition is taken at the superhorizon regime, when ϵ is extremely small, the lowest-order solution (101) suffices to calculate r_i , which is obtained by solving

$$3K_i(r_i) + r_i K_i'(r_i) = 0. \quad (112)$$

With the current choice of the functional form of $K_i(r)$, (110), the solution of (112) is given by

$$r_i^2 = 3\sigma^2 \quad \text{for } B = 0, \quad (113)$$

and

$$r_i^2 = \sigma^2 \frac{5B - 2 + \sqrt{(5B - 2)^2 + 24B}}{2B} \quad \text{for } B \neq 0. \quad (114)$$

We have obtained analytic solutions for curvature profiles with $(B, \sigma) = (1, 0.7), (0, 0.7), (1, 0.3), (0, 0.3)$, corresponding to wide and steep, wide and shallow, narrow and steep, narrow and shallow profiles, respectively. Plots of these profiles are shown in Figure 1. Note that the physical length scale in the asymptotic Friedmann region is obtained by multiplying by the scale factor $S(t)$, whose normalization we have not specified. We can therefore set up initial conditions for PBH formation with arbitrary mass scales by adjusting the normalization of $S(t)$ which appears in the expansion parameter.

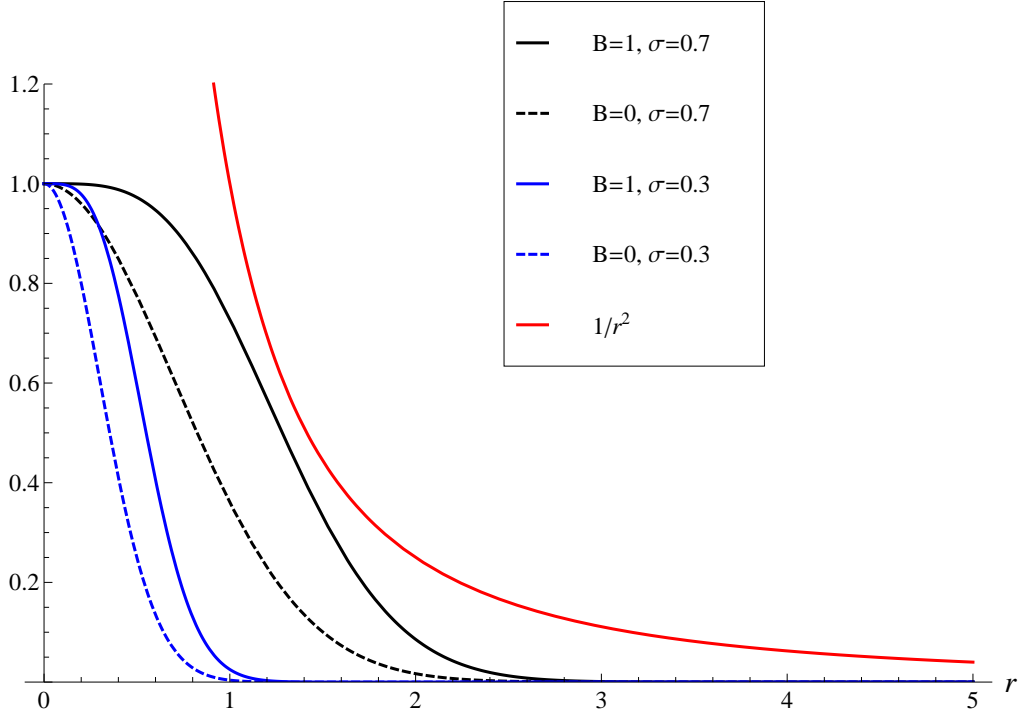


FIG. 1: Initial curvature profiles $K_i(r)$ which are used as specific examples to obtain expansion coefficients of the tilde-variables. Note that these functions have to satisfy $K_i(r) < 1/r^2$.

For these four specific profiles, expansion coefficients of the tilde-variables are calculated by solving the recurrence formulae (85), (86), (89), (91), (97) and (98) numerically. Then, the quantity ϵ_{\max} was calculated for $\Delta = 10^{-1}, 10^{-3}, 10^{-5}$ and $N = 1 - 7$. The values of ϵ_{\max} are summarized in Table I. When an asymptotic expansion of higher-order is used, ϵ_{\max} is larger, so the analytic solution constructed is sufficiently accurate until a later time. For instance, one can see from the table that when an asymptotic expansion of first order is used, the numerical calculation has to be started at $\epsilon = 0.0064$ in order to maintain the accuracy of order 10^{-5} , for the profile with $(B, \sigma) = (0, 0.7)$. On the other hand, if we use an asymptotic expansion of seventh order, we can follow the evolution of perturbation until $\epsilon = 0.51$, maintaining the accuracy of 10^{-5} , for the profile with $(B, \sigma) = (0, 0.7)$. The dependence of ϵ_{\max} on the order of the asymptotic expansion, N , is more clearly seen from Figure 2, in which the profile with $(B, \sigma) = (0, 0.7)$ is used and Δ

(B, σ)	$\Delta \backslash N$	0	1	2	3	4	5	6	7
(1, 0.7)	10^{-1}	0.070	0.30	0.64	0.73	0.84	0.93	0.98	1.0
	10^{-3}	7.0×10^{-4}	0.030	0.14	0.23	0.34	0.43	0.51	0.57
	10^{-5}	7.0×10^{-6}	0.0030	0.030	0.073	0.13	0.20	0.26	0.32
(0, 0.7)	10^{-1}	0.10	0.64	0.95	1.3	1.4	1.5	1.6	1.6
	10^{-3}	0.0010	0.064	0.21	0.41	0.56	0.70	0.82	0.91
	10^{-5}	1.0×10^{-5}	0.0064	0.044	0.13	0.22	0.32	0.42	0.51
(1, 0.3)	10^{-1}	0.38	1.4	1.1	1.1	1.3	1.5	1.6	1.7
	10^{-3}	0.0038	0.14	0.23	0.36	0.53	0.70	0.84	0.95
	10^{-5}	3.8×10^{-5}	0.014	0.049	0.11	0.21	0.33	0.44	0.53
(0, 0.3)	10^{-1}	0.56	1.2	1.6	2.1	2.5	2.8	3.2	3.0
	10^{-3}	0.0056	0.12	0.34	0.66	1.0	1.3	1.6	1.7
	10^{-5}	5.6×10^{-5}	0.012	0.074	0.21	0.40	0.60	0.85	0.94

TABLE I: Values of ϵ_{\max} that satisfies the required accuracy of Δ for each pair of (B, σ) and different orders of asymptotic expansion, N .

is set to be 10^{-1} , 10^{-3} and 10^{-5} . The time dependence of Δ for asymptotic expansion of seventh order is shown in Figure 3. Note that it is determined by the first dropped eighth order terms of the expansions in this case. When the initial curvature fluctuation is wider and its profile steeper, expansion coefficients tend to be larger, so the errors in the analytic solution are also larger.

Comparison of the time dependence of the errors associated with analytic solutions with different orders is shown in Figure 4. The profile with $(B, \sigma) = (1, 0.7)$ was used for these plots. One can see clearly that the errors with higher-order expansions are relatively small and increase more slowly than those with lower-order expansions. Plots of the tilde-variables at $\epsilon = 0.9$, calculated using the asymptotic expansion of seventh order, is shown in Figure 5. Note that errors associated with these plots are less than 10^{-3} from Figure 3.

VI. DISCUSSION AND CONCLUSION

In the present paper we have formulated a recursive method of quasi-linearization which can yield appropriate initial condition for PBH formation consistent with general relativity. The evolution of the profiles of the energy density perturbation δ are shown in Figure 6. These profiles are calculated at $\epsilon = 0.1, 0.5$ and 0.9 . One can see that the region with $\delta > 0$, which corresponds to the central overdense region, is surrounded by the underdense region with $\delta < 0$ so that (54) is satisfied.

We also introduce the averaged overdensity, denoted by $\bar{\delta}$ and defined as the energy density perturbation averaged over the overdense region as follows:

$$\bar{\delta}(t) \equiv \left(\frac{4}{3} \pi R(t, r_{\text{od}})^3 \right)^{-1} \int_0^{R(t, r_{\text{od}})} 4\pi \delta R^2 dR. \quad (115)$$

Here $r_{\text{od}}(t)$ represents the comoving radius of the overdense region, which is numerically calculated from the solution of $\delta(t, r_{\text{od}}) = 0$. It turns out that $r_{\text{od}}(t)$ is very close to r_i calculated from (112),

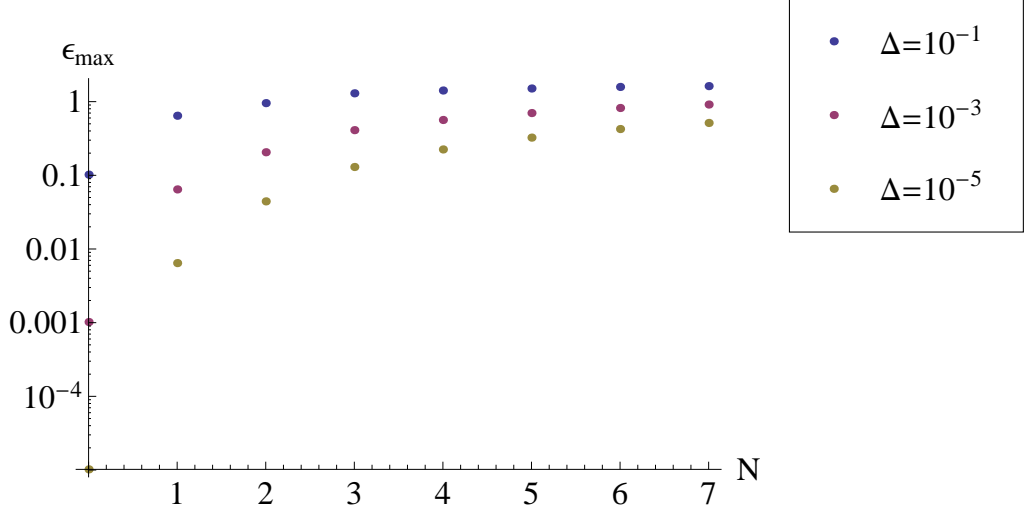


FIG. 2: The dependence of ϵ_{\max} on the order of the asymptotic expansion, N , is shown. The profile with $(B, \sigma) = (0, 0.7)$ is used.

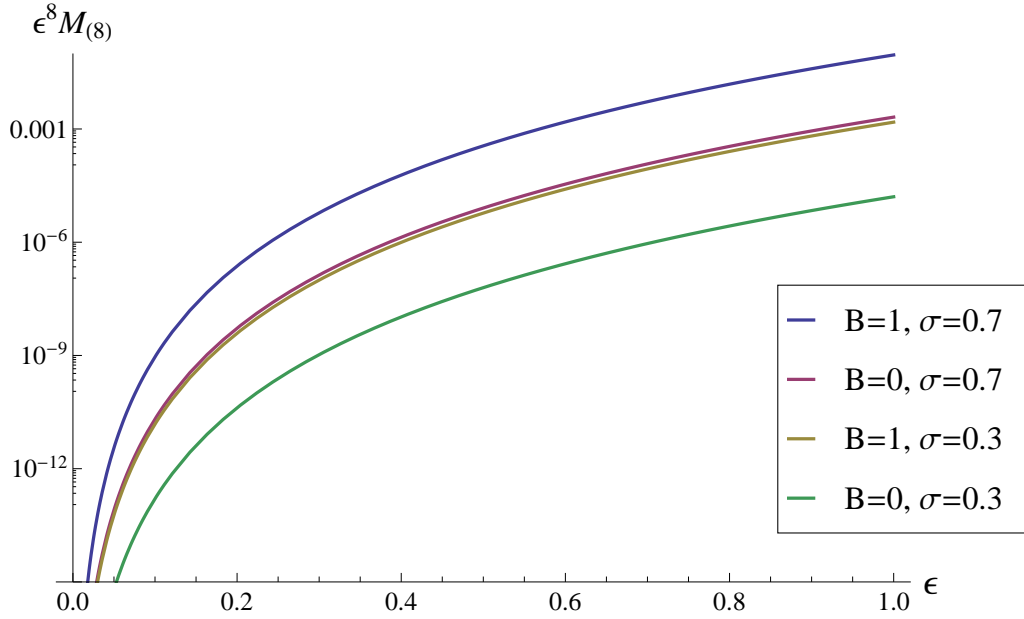


FIG. 3: The time dependence of errors associated with analytic solution obtained by asymptotic expansion of seventh order.

i.e. lowest-order expansion. This feature can be directly observed in Figure 6, where the coordinate with $\delta = 0$ hardly changes.

The time evolution of the averaged overdensity $\bar{\delta}$ is shown in Figure 7. For comparison, the results obtained using asymptotic expansions of first order are also shown. From the plots, one can confirm that higher-order corrections become more important as ϵ gets closer to unity. When the

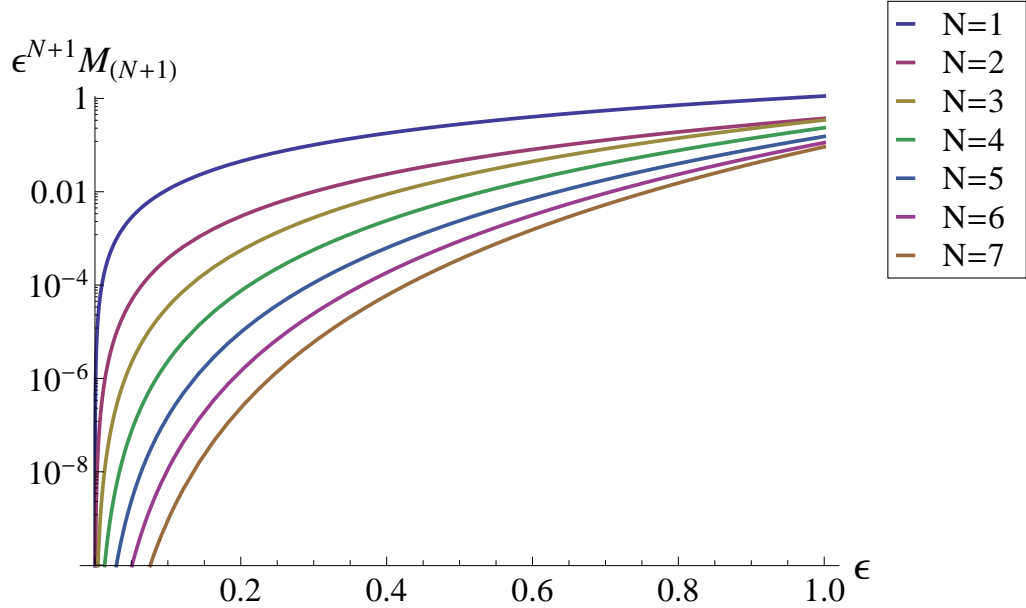


FIG. 4: Comparison of the time dependence of errors associated with analytic solutions obtained by asymptotic expansions of different orders. The profile with $(B, \sigma) = (1, 0.7)$ was used for these plots.

amplitude of initial curvature fluctuation is wider and its profile steeper, the density perturbation in the central region becomes larger, so that $\bar{\delta}$ tends to be larger. Therefore, it is more likely that wider and steeper initial curvature profiles lead to PBH formation after the perturbed region reenters the horizon. This confirms that considering the shape of profiles is crucial in the analysis of PBH formation. In addition, comparison of the time evolution of averaged overdensity $\bar{\delta}$ for $N = 1 - 4$ is shown in Figure 8. The profile with $(B, \sigma) = (1, 0.7)$ was used for these plots. When $\epsilon \ll 1$, the plots coincide well with each other, but as ϵ becomes larger, calculations using lower-order expansions start to deviate from those using higher-order ones.

We have analyzed various configurations of curvature perturbations under the assumption of spherical symmetry to set up the initial condition for the numerical analysis of PBH formation in an optimal way with the help of the asymptotic expansion. In our analysis the curvature profile has a characteristic scale much larger than the Hubble radius initially, in accordance with the inflationary cosmology [37–39] which predicts formation of superhorizon-scale curvature perturbations [40–43]. This includes those perturbations which could lead to PBH formation [44–57]. In a future paper we plan to calculate the probability of realization of the curvature profiles discussed above. Then we will eventually be able to relate the mass spectrum of PBHs with the parameters of inflationary models.

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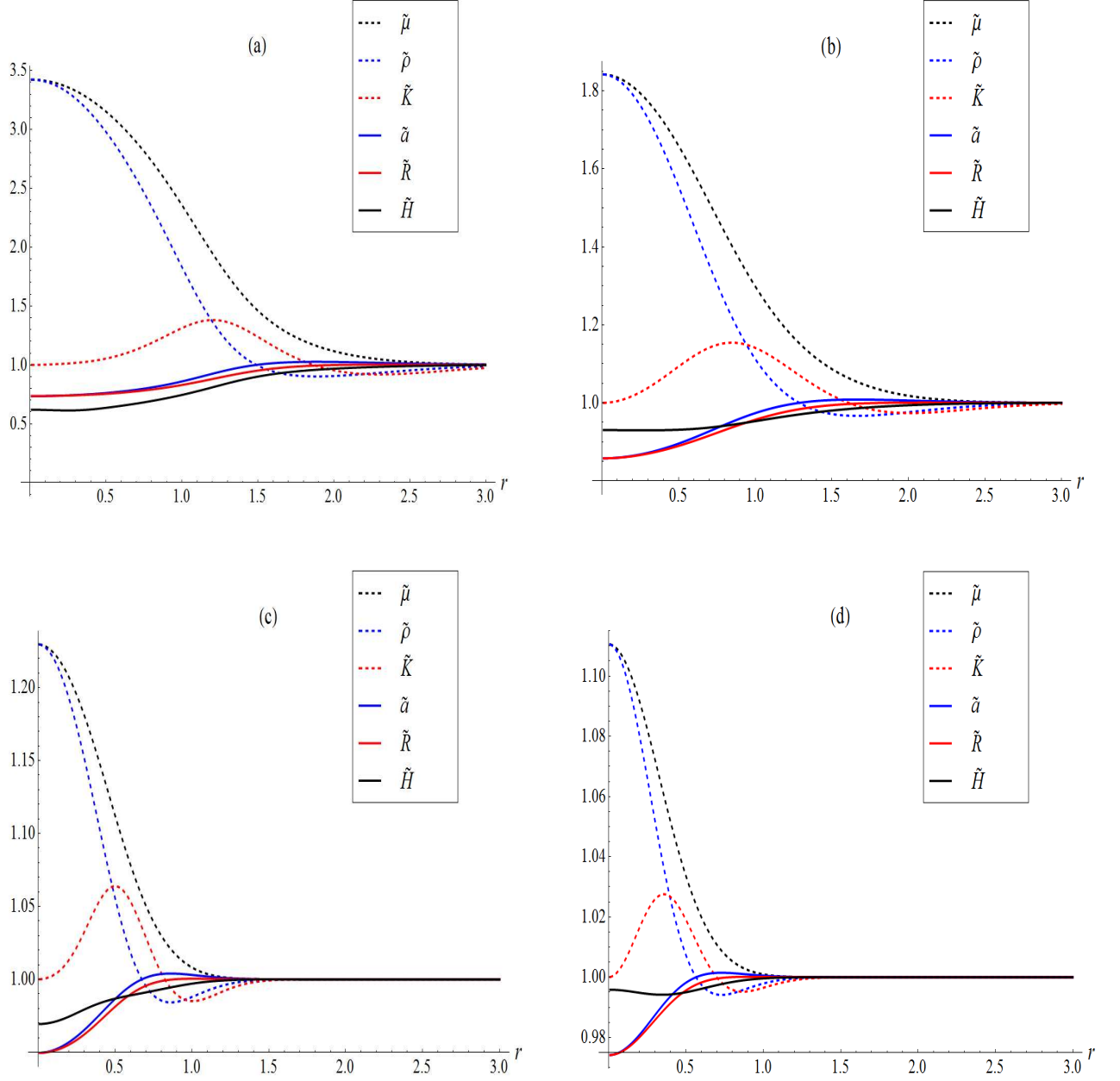


FIG. 5: Profiles of the tilde-variables at $\epsilon=0.9$, which were calculated from an asymptotic expansion of seventh order. (a), (b), (c) and (d) were obtained from $(B, \sigma) = (1, 0.7), (0, 0.7), (1, 0.3)$, and $(0, 0.3)$, respectively. Note that the errors associated with these profiles are less than of order 10^{-3} from Figure 3.

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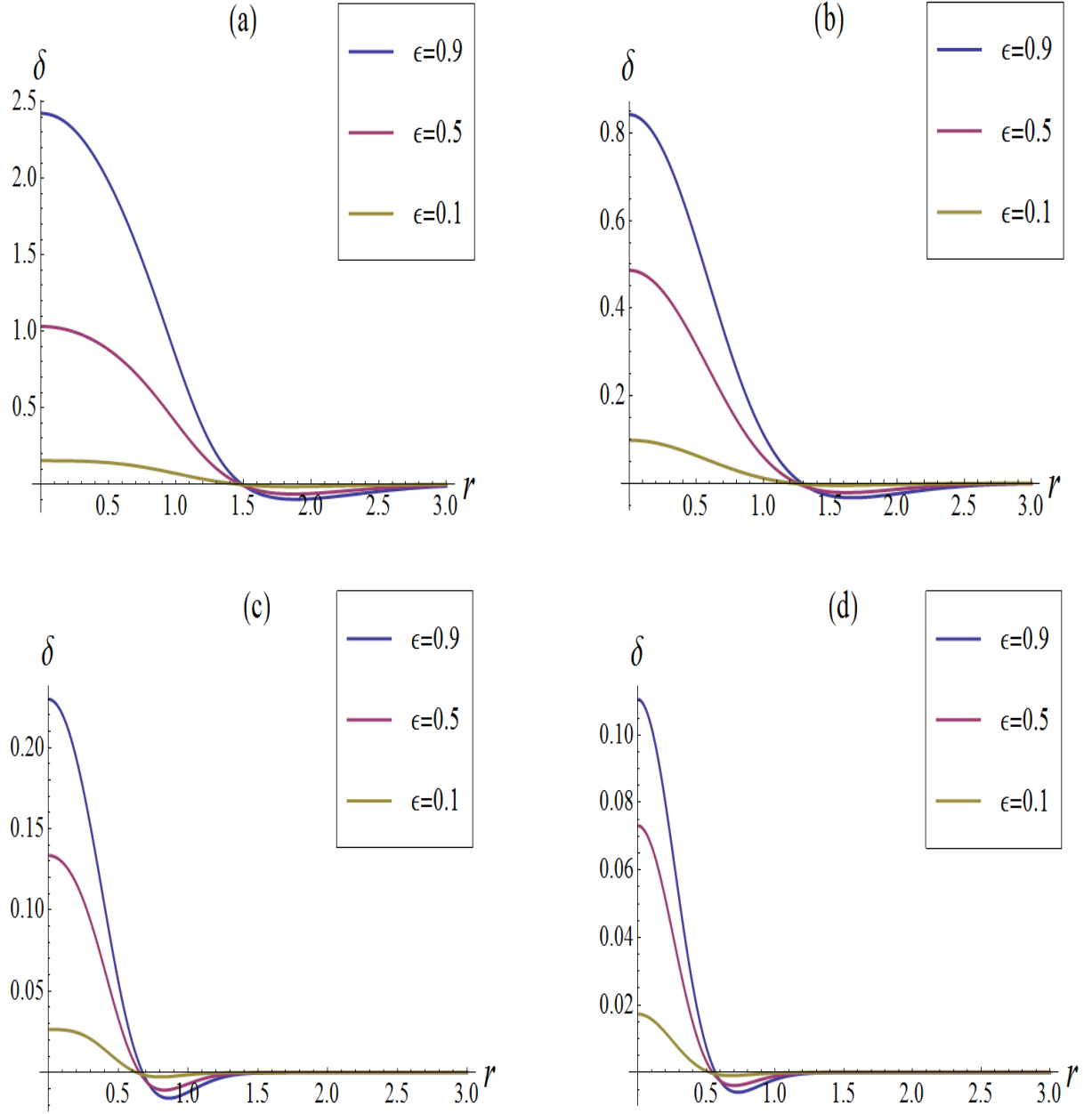


FIG. 6: An illustration of “time evolution” of the density perturbation profiles. These were calculated when $\epsilon = 0.1, 0.5$ and 0.9 . (a), (b), (c) and (d) were obtained from $(B, \sigma) = (1, 0.7), (0, 0.7), (1, 0.3)$, and $(0, 0.3)$, respectively. One can see that the region with $\delta > 0$, which corresponds to the central overdense region, is surrounded by the underdense region with $\delta < 0$.

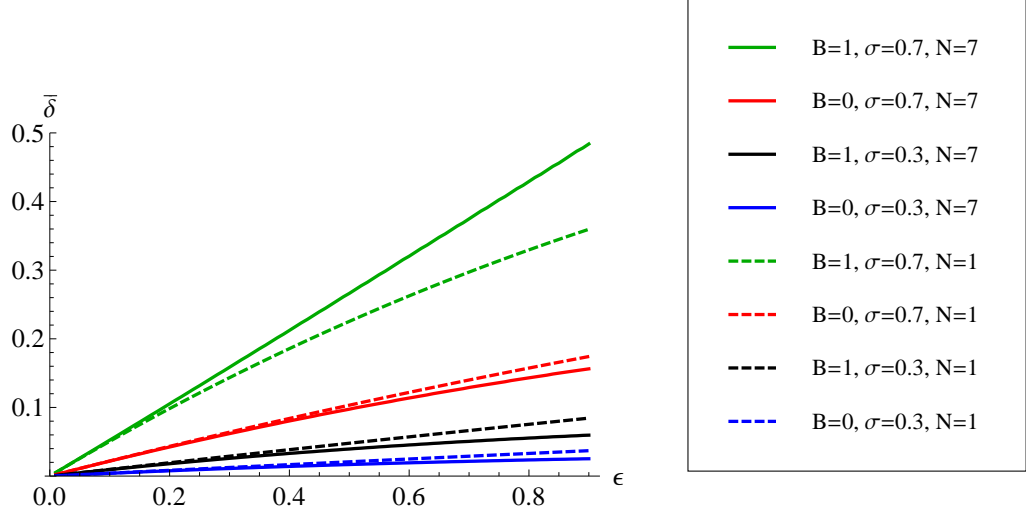


FIG. 7: Time evolution of the averaged overdensity $\bar{\delta}$ for each of the initial curvature profiles. For comparison, the results obtained from the first-order asymptotic expansion are also shown by the dashed lines.

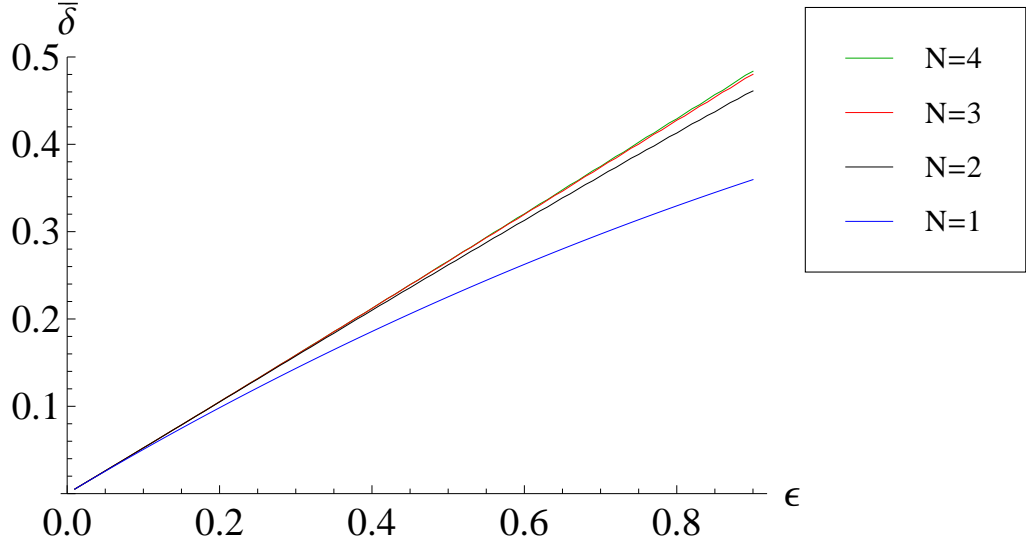


FIG. 8: Comparison of the time evolution of the averaged overdensity $\bar{\delta}$ for $N = 1 - 4$. The profile with $(B, \sigma) = (1, 0.7)$ was used for these plots.

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